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The Crystal and Molecular Structure of Diaquotris(acetylacetonato)lanthanum(III)[1]

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The crystal structure of diaquotris(acetylacetonato)lanthanum(III), $La(C_5H_7O_2)_3(H_2O)$, has been determined by three-dimensional X-ray methods. Two molecules crystallize in a triclinic unit cell of symmetry $P\bar{1}$ and dimensions a = 9.044 (7) Å, b = 11.456 (12) Å, c = 10.724 (23) Å, α = 95.57 (15)°, β = 114.66 (4)°, γ = 100.28 (10)°. A total of 2953 independent observed intensities from two crystals were measured by counter methods. The structure was refined by the method of least squares to give residuals of 0.091 and 0.059 for the two crystals. Each lanthanum ion is surrounded by eight oxygen atoms, contributed by three acetylacetonate rings and two water molecules, arranged at the vertices of a distorted square antiprism. The molecules are linked in chains by hydrogen bonds.

Introduction

A number of hydrates and adducts of rare earth acetylacetonates have been prepared and characterized,[4] and we have previously reported the structure of tris(acetylacetonato)yttrium(III) trihydrate.[5] Dihydrates have been prepared of the chelates of lanthanum, praseodymium, neodymium, and samarium, and powder patterns indicate that these crystalline compounds are isostructural.[4] This study of the structure of diaquotris(acetylacetonato)lanthanum(III) was undertaken as part of a study of solvates of rare earth chelates investigating the types of coordination of the rare earth ions, the nature of hydrogen bonding, and the correlation of the structures with the chemical and physical properties.

Experimental Section

Lanthanum acetylacetonate, prepared by a slight modification of the method of Stites, McCarty and Quill,[6] was recrystallized from a 60% ethanol-water mixture. The dihydrate was prepared by recrystallizing this product from 95% ethanol. The amount of water present in the complex was determined by Karl Fischer titrations.[4]

A crystal of dimensions 0.23 × 0.14 × 0.14 mm was sealed in a glass capillary, and approximate unit cell dimensions and the diffraction symmetry were obtained from oscillation, Weissenberg, and precession photographs. Accurate unit cell dimensions and the intensity data were measured manually on a General Electric XRD-3 X-ray spectrometer equipped with a single-crystal orienter and a scintillation counter. The intensities of all reflections for which 2θ was less than 50° were measured at a takeoff angle of 4° by the stationary-crystal, stationary-counter technique using Zr-filtered Mo Kα radiation and 40-sec counts. The settings were calculated for the Kα_1 line (λ 0.70930 Å), and factors for conversion to integrated intensities were based upon several intensities measured by a manual ω scan. The crystal was oriented about the $a^* + b^*$ direction, which makes an angle of 18° with the long dimension of the crystal. Background corrections were obtained by interpolation from a plot of intensity *vs.* angle, constructed from measurements made with the crystal out of reflecting position. No corrections were made for absorption (μ = 22.7 cm^{-1}), extinction, or anomalous dispersion. The maximum variation in the ratio of any two intensities due to absorption is about 16% for the crystals used. Corrections for instrumental variations in intensity were based upon frequent remeasurement of a few reflections; the maximum variation in intensity was 18%.

Difficulties in maintaining alignment during the course of the measurements led to the use of a second crystal, which had dimensions 0.28 × 0.12 × 0.09 mm. A total of 1969 intensities, of which 1559 were at least 7% above background and were therefore classified as observed, were recorded from the first crystal, and 1636 intensities, of which 1394 were observed, were recorded from the second crystal. Of the observed reflections, 44 were measured on both crystals, and these were used for scaling the two data sets. The mean unit cell dimensions at 25°, based on Mo Kα radiation (λ 0.7107 Å), were a = 9.044 ± 0.007 Å, b = 11.456 ± 0.012 Å, c = 10.724 ± 0.023 Å, α = 95.57 ± 0.15°, β = 114.66 ± 0.04°, γ = 100.28 ± 0.10°. The crystals remained nearly suspended in carbon tetrachloride (density 1.594 g cm^{-1}); the calculated density for two molecules pr unit cell is 1.609 g cm^{-3}.

Structure Determination and Refinement

Trial lanthanum positions were deduced from the three-dimensional Patterson function. Space group $P\bar{1}$ was assumed (and was ultimately confirmed by the structure). The metal ions occupy the general positions with $x = 0.225$, $y = 0.375$, $z = 0.225$. The contribution of La^{3+} to the structure factors was computed, and a Fourier synthesis was based upon the calculated signs and observed magnitudes of the 2583 terms for which $|F_c| \geq 0.40|F_o|$. Successive Fourier and difference Fourier calculations revealed the positions of the oxygen and carbon atoms.

The availability of data from two crystals provided the opportunity of obtaining an internal check on the accuracy of the methods used. Also, since there was no convenient way to assign relative weights to the two sets of intensities, it was decided to refine the data from the two crystals separately. A local IBM 360 adaptation of the least-squares program of Busing, Martin, and Levy[7] was used. The refinement for each crystal included a scale factor, positional parameters for the lanthanum ion and for 8 oxygen and 15 carbon atoms, anisotropic temperature factors for the lanthanum

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TABLE I

OBSERVED AND CALCULATED STRUCTURE FACTORS (×10) FOR THE OBSERVED DATA

CRYSTAL 1

K	L	FO	FC
H= -9			
0	10	70	76
1	10	108	-94
2	9	47	-52
3	9	101	99
H= -8			
-5	9	72	80
-5	10	87	-77
-4	9	122	-115
-3	9	114	104
-3	10	57	62
-3	11	45	-59
-2	9	97	-86
-2	10	99	-88
-1	10	109	94
-1	11	27	52
0	9	85	68
0	10	75	-95
0	11	44	-64
1	9	124	-120
1	11	55	58
2	8	45	-70
2	10	34	73
H= -7			
-8	8	116	120
-7	8	120	-118
-7	9	60	-66
-6	8	24	47
-6	9	148	120
-5	8	47	56
-5	9	115	-111
-5	10	53	-59
-4	8	101	-107
-4	10	82	74
-3	8	146	131
-3	11	26	-57
-2	8	167	-149
-2	9	122	-101
-2	11	60	65
-1	9	150	142
-1	12	50	-44
0	8	137	144
1	8	171	-153
1	11	41	55
1	12	39	-48
2	7	89	-106
H= -6			
-9	7	28	-62
-9	8	103	103
-8	7	154	151
-8	9	101	-94
-7	7	141	-143
-7	8	88	-81
-7	9	100	87
-7	10	64	76
-6	8	109	116
-6	10	90	-112
-5	8	108	-115
-5	9	46	-58
-5	10	49	73
-5	11	27	58
-4	7	179	-169
-4	8	88	74
-4	9	104	109
-4	11	41	-61
-3	7	220	204
-3	9	131	-116
-3	10	83	-96
-3	11	54	44
-3	12	58	57
-2	7	96	-94
-2	8	159	-128
-2	10	139	150
-2	12	72	-62
-1	7	51	-69
0	7	179	166
1	7	268	-246
1	11	32	-22
2	6	103	-116
H= -5			
-10	7	113	-117
-9	6	44	-53
-9	7	131	129
-9	8	84	87
-8	6	89	135
-8	8	127	-117
-8	10	91	70
-7	6	148	-163
-7	7	66	-87
-7	8	69	73
-7	9	37	74
-7	11	38	-53
-6	6	137	123
-6	7	185	171
-6	9	111	-120
-5	7	252	-224
-5	8	128	-125
-5	9	99	101
-5	10	101	113
-5	11	25	-29
-5	12	52	-48
-4	6	230	-213
-4	7	146	145
-4	8	225	233
-4	10	135	-146
-4	12	61	54
-3	6	214	222
-3	8	147	-150
-3	9	97	-118
-3	10	106	117
-3	11	89	106
-2	6	90	-89
-2	7	131	-119
-2	8	65	61
-2	9	119	128
-2	11	99	-89
-2	12	26	-9
-1	8	18	36
-1	10	25	-24
0	6	227	242
1	5	107	-111
1	6	209	-201
1	9	23	25
2	5	56	-60
H= -4			
-11	5	109	123
-11	6	70	76
-11	7	54	-89
-10	5	44	-56
-10	6	128	-133
-10	8	59	100
-9	6	127	132
-9	7	62	73
-9	8	65	-82
-9	9	47	-80
-8	5	175	186
-8	7	157	-148
-8	9	85	94
-7	5	275	-273
-7	6	191	-172
-7	7	77	72
-7	8	124	133
-7	9	76	-99
-7	10	39	-61
-6	5	152	159
-6	6	281	260
-6	8	191	-200
-6	10	77	80
-5	5	34	23
-5	6	228	-221
-5	7	85	-96
-5	8	179	175
-5	9	130	132
-5	10	49	-37
-5	11	55	-49
-4	5	265	-249
-4	6	192	184
-4	7	157	153
-4	8	59	-78
-4	9	130	-138
-4	11	69	47
-3	5	642	414
-3	6	39	-38
-3	7	179	-169
-3	8	82	-73
-3	9	41	51
-3	10	73	88
-3	12	35	-44
-2	5	220	-216
-2	6	163	-151
-2	7	142	141
-2	8	135	115
-2	9	32	22
-2	10	109	-95
-1	5	144	149
-1	12	26	-18
0	5	34	52
1	4	145	-141
1	10	32	-37
H= -3			
-12	4	94	-121
-11	4	92	125
-11	5	40	73
-11	6	113	-112
-11	7	50	-98
-10	4	45	-69
-10	5	166	-168
-10	7	104	141
-10	9	65	-87
-9	4	109	-105
-9	5	131	144
-9	6	142	123
-9	7	106	-136
-9	8	84	-93
-9	10	65	85
-8	4	205	206
-8	5	106	-117
-8	6	190	-220
-8	8	160	147
-8	10	62	-54
-7	4	259	-274
-7	5	24	-52
-7	6	148	149
-7	7	133	126
-7	8	83	-89
-7	9	87	-77
-7	11	75	66
-6	4	213	209
-6	5	156	152
-6	6	88	-78
-6	7	138	-135
-6	9	92	83
-6	11	36	-30
-5	5	209	-192
-5	6	29	-21
-5	7	125	114
-5	8	85	77
-5	9	48	-36
-5	10	80	-67
-5	12	51	55
-4	4	274	-284
-4	5	226	214
-4	6	143	137
-4	7	43	-42
-4	8	137	-128
-4	9	49	-50
-4	10	99	99
-3	4	467	458
-3	5	19	-42
-3	6	297	-294
-3	7	101	-119
-3	8	60	53
-3	9	103	114
-3	10	41	-52
-3	11	59	-59
-2	4	381	-362
-2	5	256	-266
-2	6	187	180
-2	7	206	210
-2	9	144	-153
-2	11	70	58
-1	4	104	101
-1	5	309	285
-1	6	74	81
1	3	200	-211
H= -2			
-12	3	133	-143
-12	5	159	140
-11	3	89	132
-11	4	99	104
-11	5	129	-124
-11	6	80	-112
-11	7	42	67
-11	8	51	67
-10	3	118	-128
-10	4	193	-192
-10	6	149	163
-10	8	64	-60
-9	4	232	221
-9	5	73	83
-9	6	94	-106
-9	7	58	-83
-9	9	102	112
-8	3	105	123
-8	4	238	-230
-8	5	149	-161
-8	7	129	144
-8	9	44	-62
-8	10	26	-48
-7	3	249	-249
-7	4	66	67
-7	5	156	164
-7	6	100	111
-7	7	109	-95
-7	8	144	-135
-7	10	71	63
-6	3	293	276
-6	4	198	203
-6	6	136	-137
-6	8	166	184
-6	10	38	-38
-6	11	58	-66
-5	4	298	-284
-5	5	51	-68
-5	6	196	177
-5	7	85	76
-5	8	101	-102
-5	9	97	-97
-5	11	77	62
-4	3	358	-338
-4	4	164	161
-4	5	221	222
-4	6	184	-179
-4	7	182	-177
-4	9	143	142
-4	11	59	-77
-4	12	28	-46
-3	3	520	501
-3	4	156	137
-3	5	370	-373
-3	6	25	-25
-3	7	140	160
-3	8	98	117
-3	9	69	-82
-3	10	83	-76
-3	12	43	23
-2	3	542	-543
-2	4	348	-332
-2	5	167	158
-2	6	256	317
-2	7	58	85
-2	8	142	-164
-2	10	100	100
-2	11	30	17
-1	3	78	76
-1	4	323	322
-1	5	69	75
-1	6	227	-273
-1	7	150	-218
0	10	28	-32
H= -1			
-13	3	70	-105
-13	4	40	-62
-12	2	146	-140
-12	4	133	118
-12	6	49	-88
-11	2	172	189
-11	4	89	-88
-11	5	84	-94
-11	7	79	54
-10	2	166	-163
-10	3	131	-139
-10	5	137	153
-10	7	55	-61
-10	8	33	-35
-10	9	50	52
-9	2	50	48
-9	3	207	212
-9	4	55	66
-9	5	109	-117
-9	6	99	-118
-9	8	93	92
-9	10	73	-54
-8	2	183	196
-8	3	160	-149
-8	4	163	-183
-8	5	19	38
-8	6	188	213
-8	8	84	-100
-8	9	53	-69
-8	10	42	35
-7	2	335	-330
-7	3	69	74
-7	4	308	321
-7	5	121	122
-7	6	158	-156
-7	7	205	-200
-7	8	55	48
-7	9	75	52
-7	11	65	-53
-6	2	279	294
-6	3	281	286
-6	4	159	-143
-6	5	251	-234
-6	6	22	39
-6	7	224	235
-6	9	91	-107
-6	10	44	-62
-5	2	70	59
-5	3	325	-326
-5	4	77	-81
-5	5	285	260
-5	6	98	83
-5	7	135	-144
-5	8	124	-137
-5	9	74	93
-5	10	68	57
-4	2	210	-205
-4	4	286	264
-4	5	98	-84
-4	6	186	-192
-4	8	159	170
-4	9	39	28
-4	10	104	-113
-4	11	45	-29
-3	2	397	410
-3	3	85	84
-3	4	343	-325
-3	5	69	-71
-3	6	152	155
-3	7	122	140
-3	8	88	-104
-3	9	120	-112
-3	10	39	49
-3	11	54	58
-2	2	582	-577
-2	3	230	-239
-2	4	342	344
-2	5	316	356
-2	6	38	55
-2	7	141	-168
-2	9	98	77
-2	10	39	57
-2	11	47	-35
-2	12	38	-45
-1	2	106	-94
-1	3	561	502
-1	4	36	48
-1	5	354	-405
-1	6	83	-90
-1	7	159	166
-1	8	91	105
0	9	25	-37
1	11	43	-30
H= 0			
-13	2	74	-93
-13	4	57	69
-12	1	101	-111
-12	5	80	-106
-12	7	53	80
-11	1	174	177
-11	3	99	-116
-11	4	111	-121
-11	5	51	74
-11	6	79	83
-11	8	70	-71
-10	1	74	-95
-10	4	201	205
-10	6	99	-100
-10	8	75	67
-10	9	65	53
-9	3	83	83
-9	4	159	-169
-9	5	146	-141
-9	6	101	86
-9	7	69	71
-9	9	75	-72
-8	1	227	225
-8	3	252	-244
-8	4	67	62
-8	5	181	183
-8	7	178	-203
-8	8	46	-47
-8	9	45	39
-8	10	37	25
-7	2	34	46
-7	3	334	333
-7	4	122	116
-7	5	159	-146
-7	6	218	-227
-7	7	126	122
-7	8	92	63
-7	10	75	-34
-6	2	240	223
-6	3	119	-96
-6	4	283	-276
-6	6	224	238
-6	7	74	78
-6	8	117	-114
-6	9	28	-43
-5	2	459	-449
-5	3	265	-249
-5	4	219	214
-5	5	110	101
-5	6	150	-159
-5	7	124	-136
-5	8	45	18
-5	9	113	100
-5	11	55	-49
-4	2	264	254
-4	3	398	367
-4	4	226	-234
-4	5	218	-219
-4	6	28	40
-4	7	101	90
-4	8	49	80
-4	9	98	-93
-4	10	66	-62
-3	1	398	357
-3	2	82	61
-3	3	488	-463
-3	4	189	195
-3	5	296	324
-3	6	122	138
-3	7	112	-114
-3	8	97	-83
-3	9	42	62
-3	10	94	86
-2	1	292	-279
-2	2	243	-246
-2	3	403	414
-2	4	96	112
-2	5	197	-228
-2	6	177	-204
-2	8	126	129
-2	10	53	-34
-2	11	42	-25
-1	1	382	364
-1	2	378	376
-1	3	120	-131
-1	4	275	-310
-1	5	56	-63
-1	6	137	151
-1	7	97	99
-1	8	99	-108
-1	9	95	-86
0	10	39	23
1	9	48	-53
H= 1			
-13	-1	97	98
-13	1	102	-120
-13	2	37	-63
-13	3	84	95
-13	4	57	79
-12	0	111	-117
-12	2	122	140
-12	3	23	-28
-12	4	134	-132
-12	6	88	95
-11	0	216	213
-11	2	144	-158
-11	3	128	-118
-11	4	136	130
-11	5	105	105
-11	6	39	-54
-11	7	85	-75
-10	0	117	-129
-10	2	71	72
-10	3	186	184
-10	5	286	-198
-10	7	77	73
-10	8	53	47
-9	-1	214	-204
-9	1	204	196
-9	2	73	73
-9	3	154	-155
-9	4	131	-134
-9	5	114	120
-9	6	86	90
-9	7	48	-61
-9	8	80	-68
-8	1	108	-105
-8	2	232	-221
-8	3	93	73
-8	4	108	111
-8	5	21	39
-8	6	175	-179
-8	7	43	-51
-8	8	66	69
-8	9	35	51
-7	1	100	-92
-7	2	279	277
-7	3	59	49
-7	4	160	-142
-7	5	118	-116
-7	6	66	73
-7	7	138	130
-7	8	27	-11
-7	9	96	-77
-6	1	251	248
-6	2	339	-324
-6	3	328	-313
-6	5	188	177
-6	6	62	80
-6	7	87	-69
-6	9	49	48
-6	10	63	68
-5	1	585	-558
-5	2	53	-59
-5	3	372	353
-5	4	179	156
-5	5	174	-179
-5	6	76	-69
-5	7	59	59
-5	8	107	103
-5	10	60	-47
-4	0	22	37
-4	1	364	381
-4	2	223	226
-4	3	394	-358
-4	4	240	-256
-4	6	127	143
-4	8	99	-71
-3	0	189	195
-3	1	158	-127
-3	2	320	-295
-3	3	193	206
-3	4	283	308
-3	5	126	131
-3	6	120	-128
-3	7	147	-153
-3	8	62	52
-3	9	78	57
-3	11	62	-26
-2	0	558	-542
-2	1	125	-126
-2	2	352	343
-2	3	71	48
-2	4	321	-358
-2	5	159	-175
-2	6	24	24
-2	7	201	213
-2	8	60	60
-2	9	76	-50
-2	10	54	-39
-1	-1	436	-449
-1	0	654	695
-1	1	389	399
-1	2	117	-127
-1	3	342	-386
-1	4	108	-114
-1	5	188	236
-1	6	65	46
-1	7	130	-134
-1	8	164	-166
-1	10	108	79
0	-1	634	680
0	0	135	134
1	9	103	-63
H= 2			
-13	-2	104	110
-13	0	112	-125
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-7	2	92	-99
-7	3	47	58
-6	-8	69	65
-6	-7	142	138
-6	-5	146	-156
-6	-4	84	-62
-6	-3	84	83
-6	-2	166	161
-6	0	116	-121
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-5	-7	85	-76
-5	-6	66	-81
-5	-5	136	137
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-5	3	76	-75
-4	-8	96	-87
-4	-6	164	156
-4	-4	189	-197
-4	-3	57	-67
-4	-2	120	118
-4	-1	161	152
-4	0	126	-110
-4	1	151	-133
-4	3	101	78
-3	-8	134	123
-3	-7	57	57
-3	-6	103	-106
-3	-5	118	-122
-3	-4	90	86
-3	-3	197	204
-3	-2	80	-77
-3	-1	281	-232
-3	0	63	-65
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-3	2	84	81
-3	3	37	-49
-2	-8	60	-70
-2	-7	138	-127
-2	-6	84	88
-2	-5	237	236
-2	-4	114	99
-2	-3	204	-214
-2	-2	98	-109
-2	-1	180	162
-2	0	127	137
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-2	2	160	-138
-1	-7	187	160
-1	-6	94	98
-1	-5	201	-194
-1	-4	244	-233
-1	-3	107	109
-1	-2	209	214
-1	0	149	-162
-1	1	43	-62
-1	2	142	119
-1	3	79	65
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0	-7	54	-56
0	-6	207	-206
0	-4	271	270
0	-2	199	-203
0	-1	149	-182
0	0	102	111
0	1	159	143
0	2	70	-66
0	3	132	-100
H= 9			
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-8	-7	98	-96
-8	-5	56	65
-8	-4	73	85
-8	-3	59	-64
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-7	-7	60	75
-7	-6	67	78
-7	-5	52	-55
-7	-4	124	-126
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-6	-6	119	-122
-6	-5	32	-41
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-6	-3	83	83
-6	-2	98	-98
-6	-1	128	-115
-6	1	88	89
-5	-8	62	-61
-5	-7	64	-85
-5	-6	23	56
-5	-5	156	146
-5	-4	60	-77
-5	-3	140	-137
-5	-1	126	130
-5	1	79	-79
-4	-9	95	-83
-4	-7	176	160
-4	-6	55	42
-4	-5	162	-157
-4	-4	54	-67
-4	-3	107	111
-4	-2	63	92
-4	-1	117	-108
-4	0	140	-126
-3	-9	94	99
-3	-8	38	50
-3	-7	154	-165
-3	-6	155	-140
-3	-5	106	97
-3	-4	153	157
-3	-2	164	-168
-3	0	131	125
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-2	-9	47	-52
-2	-8	125	-118
-2	-7	76	67
-2	-6	209	191
-2	-4	204	-199
-2	-3	112	-120
-2	-2	127	134
-2	-1	144	136
-2	0	45	-61
-2	1	131	-118
-1	-8	133	126
-1	-6	162	-161
-1	-5	115	-147
-1	-4	130	128
-1	-3	178	192
-1	-1	141	-145
-1	0	53	-54
-1	1	138	121
0	-9	99	64
0	-8	65	-79
0	-7	83	-105
0	-5	117	167
0	-3	153	-176
0	-2	108	-114
0	-1	82	96
0	0	163	153
H= 10			
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-7	-3	129	120
-6	-7	83	-83
-6	-5	112	115
-6	-4	38	55
-6	-3	84	-93
-6	-2	113	-108
-5	-8	73	-74
-5	-7	45	68
-5	-6	115	102
-5	-5	28	-51
-5	-4	93	-108
-5	-2	124	128
-4	-8	116	103
-4	-6	134	-133
-4	-5	54	-51
-4	-4	61	69
-4	-3	77	85
-4	-2	82	-88
-4	-1	116	-115
-3	-8	114	-100
-3	-7	58	-77
-3	-6	82	91
-3	-5	108	119
-3	-3	122	-121
-3	-1	125	126
-2	-9	66	-66
-2	-7	60	99
-2	-5	120	-138
-2	-4	38	-65
-2	-3	111	121
-2	-2	136	124
-1	-9	92	93
-1	-7	83	-100
-1	-6	112	-118
-1	-5	58	88
-1	-4	128	144
-1	-2	124	-133
0	-9	64	-78
0	-8	84	-94
0	-6	141	151
0	-4	142	-156
0	-3	88	-86
0	-2	98	102

CRYSTAL 2

K	L	FO	FC
H= -9			
2	10	73	78
4	9	103	-114
4	10	82	-89
6	9	62	62
H= -8			
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3	8	142	147
3	10	87	-94
4	8	116	-118
4	9	74	-107
4	10	63	65
4	11	71	88
5	9	151	156
6	8	70	84
6	9	76	-82
6	10	56	-73
7	8	103	-100
8	8	63	75
H= -7			
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0	9	98	-129
0	10	164	-153
0	12	149	141
1	10	128	123
2	8	151	156
2	9	147	135
2	11	121	-125
3	7	159	162
3	9	170	-157
3	11	103	117
4	7	107	-112
4	8	40	-111
4	9	105	125
4	10	101	112
4	11	66	-78
5	7	30	62
5	8	132	137
5	10	147	-143
6	7	35	39
6	8	106	-111
6	9	75	-87
6	10	52	71
7	7	155	-163
7	9	87	85
8	7	146	148
8	9	75	-85
9	7	94	-104
9	8	87	-106
H= -6			
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-1	9	92	92
-1	10	141	-147
-1	12	107	120
0	8	88	-101
0	9	190	-175
0	11	124	133
1	9	202	191
1	10	75	92
1	12	89	-105
2	7	257	273
2	8	217	223
2	9	64	-81
2	10	145	-137
3	6	139	124
3	7	75	-70
3	8	217	-222
3	10	148	158
3	11	47	65
4	6	174	-185
4	7	47	-76
4	8	126	116
4	9	87	101
4	10	80	-103
4	11	108	-125
5	6	120	135
5	7	145	145
5	9	141	-146
5	11	91	99
6	7	172	-185
6	8	66	-82
6	9	124	118
6	10	106	108
7	6	226	-242
7	7	34	45
7	8	104	106
7	10	97	-118
8	6	199	203
8	8	95	-90
8	9	67	-72
9	6	60	-96
9	7	76	-89
10	7	94	105
H= -5			
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0	7	174	-176
0	8	182	-186
0	9	82	95
0	10	89	112
0	12	119	-142
1	8	252	260
1	10	100	-98
1	11	123	-136
2	6	280	277
2	7	188	188
2	8	113	-106
2	9	155	-167
2	11	139	147
3	5	252	255
3	6	130	-136
3	7	246	-242
3	9	161	160
3	10	63	80
3	11	71	-89
4	5	301	-302
4	6	61	-65
4	7	165	165
4	8	158	173
4	9	115	-119
4	10	159	-147
5	5	174	157
5	6	173	178
5	8	215	-222
5	10	148	142
5	11	32	71
6	6	200	-198
6	7	61	-63
6	8	149	141
6	9	107	112
6	10	39	-64
7	5	150	-168
7	6	111	116
7	7	134	129
7	9	108	-106
8	5	215	211
8	7	88	-97
8	8	51	-66
9	5	54	-71
9	6	46	-69
9	7	63	57
9	8	98	103
10	6	90	97
10	7	30	33
11	6	33	-98
H= -4			
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-1	8	214	-210
-1	9	108	-127
-1	10	94	92
-1	11	119	138
0	6	222	-212
0	7	234	-237
0	8	145	144
0	9	169	161
0	11	197	-209
1	5	269	-268
1	7	297	293
1	9	163	-168
1	11	110	116
1	12	181	114
2	4	127	-114
2	5	290	283
2	6	224	226
2	7	193	-190
2	8	197	-205
2	9	24	51
2	10	170	189
3	4	345	340
3	5	178	-172
3	6	366	-366
3	7	39	-55
3	8	167	174
3	9	69	69
3	10	117	-126
3	11	77	-96
3	12	38	59
4	6	388	-335
4	5	32	-20
4	6	164	144
4	7	177	183
4	8	126	-136
4	9	140	-143
4	11	116	125
5	4	249	254
5	5	198	212
5	7	166	-156
5	9	183	189
5	10	44	60
5	11	53	-81
6	4	59	-73
6	5	222	-231
6	6	82	-84
6	7	90	87
6	8	137	151
6	9	70	-71
6	10	135	-117
7	4	61	-70
7	5	166	163
7	6	177	177
7	8	187	-176
7	9	76	-97
7	10	116	110
8	4	224	225
8	5	40	41
8	6	160	-142
8	7	27	-30
8	8	97	106
8	9	105	116
9	4	106	-101
9	5	117	-107
9	6	63	77
9	7	107	112
9	8	29	-51
10	5	113	123
10	7	113	-107
11	4	44	75
11	5	63	-84
11	6	85	-103
12	4	110	-101
H= -3			
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-1	8	90	-93
-1	9	161	164
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0	4	73	73
0	5	305	-302
0	6	325	-324
0	7	148	162
0	8	245	237
0	10	180	-200
0	12	140	138
1	4	344	-342
1	5	61	51
1	6	347	324
1	8	214	-214
1	9	154	-150
1	10	132	150
1	11	170	171
2	3	33	-12
2	4	177	163
2	5	110	107
2	6	301	-293
2	7	183	-181
2	8	75	69
2	9	268	263
2	11	155	-142
3	3	385	398
3	4	100	-102
3	5	228	-210
3	6	94	-100
3	7	223	218
3	8	36	38
3	9	201	-195
3	10	123	-104
3	11	91	98
4	3	423	-424
4	4	64	-69
4	5	98	79
4	6	271	265
4	7	53	-77
4	8	178	-170
4	9	57	82
4	10	91	104
5	3	280	277
5	4	288	279
5	6	218	-228
5	7	79	-102
5	8	207	206
5	10	89	-98
5	11	63	-70
6	3	45	-55
6	4	324	-313
6	5	67	-61
6	6	240	251
6	7	124	125
6	8	110	-101
6	9	128	-124
7	3	117	-117
7	4	194	200
7	5	217	288
7	6	194	-197
7	7	193	-190
7	9	109	120
8	3	254	255
8	5	212	-218
8	7	143	146
8	8	59	68
8	9	68	-74
9	3	225	-203
9	4	163	-156
9	5	72	78
9	6	96	104
9	8	84	-99
10	4	113	123
10	6	98	-104
11	4	91	-95
11	5	70	-87
12	3	65	-76
H= -2			
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-3	3	525	495
-2	3	549	-547
-1	8	174	175
-1	9	170	174
-1	10	69	-72
-1	11	169	-158
0	3	86	-62
0	4	372	-354
0	5	306	-294
0	6	197	192
0	7	343	333
0	9	210	-201

TABLE I (*Continued*)

K	L	FO	FC
0	11	113	142
1	2	80	-64
1	3	55	64
1	4	55	-60
1	5	470	466
1	7	316	-305
1	8	86	-81
1	9	209	211
1	10	210	203
2	2	73	-54
2	3	60	78
2	4	167	172
2	5	261	-255
2	6	232	-228
2	7	206	203
2	8	222	221
2	10	186	-181
3	2	476	461
3	3	298	-280
3	4	309	-300
3	5	61	-81
3	6	285	283
3	7	29	17
3	8	253	-247
3	9	115	-101
3	10	90	94
3	11	121	113
4	2	577	-573
4	3	16	24
4	4	553	564
4	5	196	182
4	6	94	-92
4	7	165	-153
4	8	106	114
4	9	90	98
4	11	137	-128
5	2	260	266
5	3	300	321
5	4	268	-274
5	5	244	-245
5	6	52	54
5	7	215	214
5	9	85	-89
5	10	62	-61
6	2	41	-23
6	3	311	-326
6	4	108	-113
6	5	234	242
6	7	164	-161
6	8	131	-133
6	10	100	86
7	2	128	-129
7	3	161	169
7	4	194	194
7	5	79	-69
7	6	155	-152
7	8	140	146
8	2	209	213
8	3	45	-33
8	4	222	-221
8	5	52	-55
8	6	141	131
8	7	147	139
9	2	267	-264
9	3	152	-160
9	4	118	119
9	5	119	109
9	7	114	-119
10	3	119	116
10	5	141	-148
10	7	92	87
11	4	52	-71
11	5	64	78
12	2	51	-77
12	4	83	86
13	2	99	106
H= -1			
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-2	4	356	359
-1	3	556	533
-1	9	82	-89
-1	10	130	-138
-1	12	123	138
0	2	202	194
0	3	125	-118
0	4	401	-390
0	5	294	294
0	6	249	252
0	7	117	-110
0	8	182	-193
0	10	134	133
1	1	433	-446
1	2	196	-185
1	4	500	489
1	6	312	-301
1	8	149	160
1	9	206	196
1	10	100	-98
2	1	83	86
2	2	1079	1057
2	3	18	36
2	4	406	-376
2	5	177	-159
2	6	206	193
2	7	145	159
2	8	60	-62
2	9	214	-207
2	10	48	-49
2	11	135	116
3	1	346	349
3	2	554	-544
3	3	357	-356
3	4	381	370
3	5	330	340
3	6	47	47
3	7	267	-264
3	8	138	-122
3	9	54	71
3	10	112	106
3	11	62	-54
4	1	375	-374
4	3	498	501
4	4	49	42
4	5	198	-201
4	6	232	-235
4	7	148	151
4	8	162	147
4	10	121	-121
5	1	253	256
5	2	142	142
5	3	54	-39
5	4	198	-191
5	5	34	14
5	6	244	248
5	7	39	56
5	8	130	-141
5	9	80	-79
5	10	73	68
6	1	58	-61
6	2	256	-256
6	3	158	-146
6	4	122	137
6	5	105	104
6	6	138	-126
6	7	144	-148
6	8	82	75
6	9	152	149
7	1	113	-125
7	2	200	190
7	3	223	216
7	4	69	-83
7	5	150	-140
7	7	138	128
7	8	53	55
7	9	122	-121
8	1	137	130
8	3	260	-276
8	5	166	163
8	6	120	107
8	7	34	-49
8	8	114	-102
9	1	202	-214
9	2	106	-113
9	3	160	151
9	4	117	130
9	5	51	-50
9	6	119	-108
10	1	147	154
10	2	159	148
10	4	129	-130
10	5	34	-57
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11	4	67	77
11	5	115	106
12	1	62	-61
12	2	37	59
12	3	93	81
13	1	82	79
H= 0			
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-12	3	106	97
-10	2	124	-111
-9	2	273	254
-8	2	195	-191
-7	1	285	-307
-6	1	259	260
-5	1	198	-204
-5	2	464	-447
-4	1	63	-83
-4	3	385	373
-3	1	392	367
-3	3	502	-496
-2	1	284	-279
-2	3	429	452
-1	1	366	366
-1	2	387	392
-1	11	102	111
0	1	236	220
0	2	379	-376
0	3	214	-216
0	4	205	199
0	5	204	206
0	6	186	-176
0	7	159	-163
0	8	56	-39
0	9	196	200
0	11	104	-103
1	0	621	-658
1	1	444	-457
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1	3	518	519
1	4	131	107
1	5	316	-323
1	6	52	-49
1	7	125	119
1	8	146	138
1	10	174	-166
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2	2	21	4
2	3	492	-471
2	4	345	-365
2	5	169	155
2	6	199	186
2	7	130	-125
2	8	226	-218
2	9	25	-37
2	10	159	155
3	0	84	-79
3	1	19	-20
3	2	222	-227
3	3	268	271
3	4	332	344
3	5	116	124
3	6	300	-302
3	7	179	-177
3	8	121	114
3	9	110	105
3	10	64	-79
4	0	293	-299
4	2	320	335
4	3	79	82
4	4	182	-175
4	5	266	-264
4	6	176	167
4	7	305	286
4	9	138	-132
5	0	317	299
5	1	170	180
5	2	269	-273
5	3	276	-268
5	5	198	196
5	6	52	44
5	7	197	-197
5	8	46	-84
5	9	105	97
6	0	68	-40
6	1	279	-291
6	2	30	-33
6	3	182	188
6	4	65	66
6	5	164	-169
6	6	145	-139
6	7	93	92
6	8	150	138
7	0	21	-18
7	1	175	176
7	2	231	223
7	3	92	-82
7	4	127	-112
7	5	97	93
7	6	143	134
7	8	142	-119
8	0	142	146
8	1	28	-43
8	2	209	-210
8	3	29	-35
8	4	150	145
8	5	63	70
8	6	96	-86
8	7	106	-89
9	0	211	-219
9	1	46	-74
9	2	141	149
9	3	143	152
9	4	90	-85
9	5	168	-151
10	0	192	172
10	1	215	193
10	3	159	-152
10	4	32	-50
10	5	98	106
11	0	55	53
11	1	117	-98
11	2	31	-49
11	3	99	96
11	4	107	116
12	0	140	-129
12	2	84	86
13	0	109	104
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2	-7	103	-99
2	-5	88	93

ion, and isotropic temperature factors for the oxygen and carbon atoms. The atomic form factors used were those of Cromer, Larson, and Waber[8] for La^{3+} and those of Ibers[9] for oxygen and carbon. The values for oxygen were the average of values for the neutral atom and for O^- in order to account for the total charge of the acetylacetonate group. The contributions to the least-squares sums were weighted by $1/\sigma^2$, where σ, the standard deviation of F for each reflection, was calculated by a variation of the method of Smith and Alexander,[10] in which the contribution to the error of the correction factors, such as background measurements, the conversion of peak heights to integrated intensities, and corrections for instrumental variations were included. Unobserved data were omitted from the refinements. After these refinements, the values of the residual, $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, were 0.091 for the first crystal and 0.059 for the second crystal. The weighted residuals were 0.074 and 0.044, respectively, and the standard deviations of an observation of unit weight were 1.31 and 1.15. The largest positional parameter shift on the last cycle was about 50% of a standard deviation.

A final difference Fourier map, based on $F_o - F_c$ for all of the data, revealed three of the water hydrogen atoms. Results for the other water hydrogen and for the three methylene hydrogen atoms were inconclusive. No attempt was made to locate the hydrogen atoms on the methyl groups.

The final calculated and observed structure factors are given in Table I. The weighted average positional parameters are given in Table II.

Discussion of the Structure

Figure 1 shows one molecule of the unit cell projected along [010]. The bond lengths and angles are listed in Table III. The standard deviations of the distances

[8] D. F. Cromer, A. C. Larson, and J. T. Waber, *Acta Cryst.*, **17**, 1044 (1964).

[9] "International Tables for X-Ray Crystallography," Vol. III, The Kynoch Press, Birmingham, England, 1962, p 202.

[10] G. S. Smith and L. E. Alexander, *Acta Cryst.*, **16**, 462 (1963).

Table II

Atomic Parameters of $La(C_5H_7O_2)_3(H_2O)_2$ with Estimated Standard Deviations

Atom	x	y	z	B, Å^2
La	0.2321 (1)	0.3847 (1)	0.2179 (1)	[a]
O(1)	0.0513 (11)	0.2966 (7)	−0.0326 (14)	4.4 (6)
O(2)	0.2845 (15)	0.1922 (8)	0.1539 (17)	4.9 (3)
O(3)	−0.0053 (15)	0.2790 (8)	0.2573 (9)	4.5 (2)
O(4)	0.3307 (10)	0.2996 (8)	0.4348 (8)	3.6 (4)
O(5)	0.3110 (13)	0.5436 (11)	0.1029 (8)	3.6 (2)
O(6)	0.5423 (17)	0.4474 (7)	0.3042 (9)	4.0 (2)
O(7)	−0.0020 (9)	0.4979 (7)	0.1403 (8)	3.3 (2)
O(8)	0.3407 (9)	0.5694 (7)	0.4176 (18)	3.4 (2)
C(1)	0.0182 (18)	0.1991 (13)	−0.1234 (18)	4.2 (4)
C(2)	0.1009 (18)	0.1044 (14)	−0.0820 (19)	4.6 (6)
C(3)	0.2276 (17)	0.1067 (15)	0.0479 (15)	4.2 (3)
C(4)	0.3074 (30)	−0.0043 (12)	0.0735 (15)	5.1 (3)
C(5)	−0.1113 (19)	0.1886 (13)	−0.2699 (21)	5.6 (4)
C(6)	−0.0288 (17)	0.2017 (16)	0.3309 (15)	4.1 (3)
C(7)	0.1004 (27)	0.1582 (13)	0.4263 (19)	5.0 (3)
C(8)	0.2739 (19)	0.2060 (12)	0.4721 (14)	4.1 (4)
C(9)	0.3961 (19)	0.1480 (14)	0.5727 (18)	5.8 (4)
C(10)	−0.2144 (17)	0.1551 (12)	0.3068 (15)	5.5 (2)
C(11)	0.4399 (15)	0.6133 (16)	0.0970 (13)	3.4 (5)
C(12)	0.6072 (16)	0.6037 (17)	0.1866 (14)	4.0 (3)
C(13)	0.6464 (40)	0.5237 (27)	0.2802 (27)	3.3 (3)
C(14)	0.8323 (16)	0.5298 (11)	0.3690 (14)	4.2 (3)
C(15)	0.4191 (16)	0.7062 (18)	0.0049 (14)	4.3 (3)
H(1)	0.125	0.558	0.180	6.0
H(2)	0.450	0.590	0.430	6.0
H(3)	0.300	0.500	0.335	6.0

[a] For lanthanum the anisotropic temperature factor is of the form $\exp[-\Sigma h_i h_j \beta^{ij}$, with $\beta^{11} = 0.0084$ (4), $\beta^{22} = 0.0058$ (3), $\beta^{33} = 0.0074$ (16), $\beta^{12} = 0.0016$ (8), $\beta^{13} = 0.0034$ (10), $\beta^{23} = 0.0018$ (1).

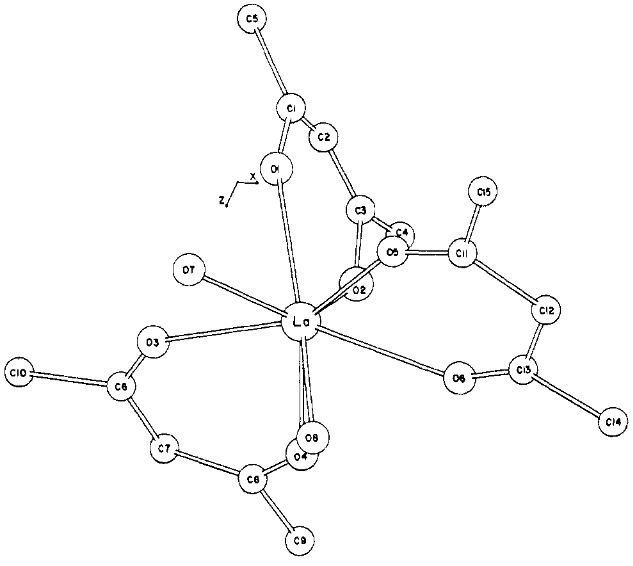

Figure 1.—Projection of one molecule along [010].

Table III

Bond Lengths and Angles

Lengths, Å		Angles, deg	
La–O(1)	2.475	O(1)–La–O(2)	69.1
La–O(2)	2.427	O(3)–La–O(4)	68.0
La–O(3)	2.487	O(5)–La–O(6)	68.5
La–O(4)	2.484	Mean	68.5 (6)
La–O(5)	2.468	O(7)–La–O(8)	76.1 (5)
La–O(6)	2.496		
Mean	2.473 (24)	La–O(1)–C(1)	141.2
La–O(7)	2.562	La–O(2)–C(3)	137.4
La–O(8)	2.584	La–O(3)–C(6)	137.4
Mean	2.573 (16)	La–O(4)–C(8)	134.7
		La–O(5)–C(11)	140.8
O(1)–C(1)	1.303	La–(6)–C(13)	137.1
O(2)–C(3)	1.274	Mean	138.1 (25)
O(3)–C(6)	1.285		
O(4)–C(8)	1.276	O(1)–C(1)–C(2)	119.6
O(5)–C(11)	1.316	O(2)–C(3)–C(2)	127.4
O(6)–C(13)	1.289	O(3)–C(6)–C(7)	123.2
Mean	1.290 (16)	O(4)–C(8)–C(7)	123.1
		O(5)–C(11)–C(12)	120.7
C(1)–C(2)	1.428	O(6)–C(13)–C(12)	126.9
C(2)–C(3)	1.389	Mean	123.5 (32)
C(6)–C(7)	1.397		
C(7)–C(8)	1.411	C(1)–C(2)–C(3)	126.3
C(11)–C(12)	1.436	C(6)–C(7)–C(8)	125.1
C(12)–C(13)	1.396	C(11)–C(12)–C(13)	125.6
Mean	1.410 (19)	Mean	125.7 (6)
C(1)–C(5)	1.483	O(1)–C(1)–C(5)	117.9
C(3)–C(4)	1.586	O(2)–C(3)–C(4)	115.4
C(6)–C(10)	1.569	O(3)–C(6)–C(10)	116.2
C(8)–C(9)	1.504	O(4)–C(8)–C(9)	118.5
C(11)–C(15)	1.517	O(5)–C(11)–C(15)	120.4
C(13)–C(14)	1.536	O(6)–C(13)–C(14)	116.0
Mean	1.532 (39)	Mean	117.4 (19)
O(7)–H(1)	1.11	C(4)–C(3)–C(2)	118.9
O(8)–H(2)	0.92	C(5)–C(1)–C(2)	121.5
O(8)–H(3)	1.02	C(9)–C(8)–C(7)	118.9
		C(10)–C(6)–C(7)	120.3
		C(14)–C(13)–C(12)	117.5
		C(15)–C(11)–C(12)	119.0
		Mean	119.4 (14)
		H(2)–O(8)–H(3)	95.4

and angles were computed by the method of Sands,[11] and these standard deviations were used in calculating the weighted averages of the distances and angles which are given in Table III. The positional parameters of the two crystals sometimes differed by several standard deviations. The anisotropic temperature factors for the lanthanum ion were also quite different for the two crystals. This comparison of the two crystals serves to illustrate the unreliability of standard deviations and temperature factors obtained by least-squares fitting of data containing systematic errors such as uncorrected absorption. In order to avoid false and misleading claims of accuracy, the standard deviations listed in Tables II–IV were based on appraisals of the variations observed between the two crystals and between chemically equivalent bonds and angles.

Each lanthanum ion is bonded to eight oxygen atoms, contributed by three bidentate acetylacetonate groups and two water molecules [O(7) and O(8)]. The average distance from a lanthanum ion to a carbonyl oxygen atom is 2.473 Å, while the average distance of lanthanum to coordinated water is 2.573 Å; the corresponding values in $Y(C_5H_7O_2)_3 \cdot 3H_2O$ were 2.366 and 2.409 Å.[5] The empirical relationship of Lingafelter and Braun,[12] based on a study of distances in acetylacetone chelates of metal ions having noble gas configurations, predicts 2.54 Å for the lanthanum–carbonyl oxygen

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(11) D. E. Sands, *Acta Cryst.*, **21**, 868 (1966).

(12) E. C. Lingafelter and R. L. Braun, *J. Am. Chem. Soc.*, **88**, 2951 (1966).

TABLE IV

DIMENSIONS OF COORDINATION POLYHEDRON

Dimensions, Å[a]

O(1)–O(2)	2.768	O(7)–O(3)	2.904	O(5)–O(7)	2.985
O(2)–O(6)	3.184	O(1)–O(3)	3.362	O(7)–O(1)	3.050
O(6)–O(5)	2.795	O(3)–O(2)	3.493	O(1)–O(6)	4.294
O(5)–O(1)	3.101	O(2)–O(4)	2.966	O(2)–O(5)	4.091
O(3)–O(4)	2.780	O(4)–O(6)	3.169	O(3)–O(8)	3.812
O(4)–O(8)	3.102	O(6)–O(8)	3.024	O(4)–O(7)	4.476
O(8)–O(7)	3.168	O(8)–O(5)	3.248		

Angles, Deg[b]

O(5)–O(1)–O(2)	87.9	O(3)–O(2)–O(4)	50.3	O(5)–O(6)–O(8)	67.7
O(1)–O(2)–O(6)	92.1	O(2)–O(4)–O(3)	74.8	O(8)–O(5)–O(7)	60.9
O(2)–O(6)–O(5)	86.4	O(4)–O(3)–O(2)	54.8	O(5)–O(7)–O(8)	63.6
O(6)–O(5)–O(1)	93.0	O(2)–O(4)–O(6)	62.3	O(7)–O(8)–O(5)	55.4
O(7)–O(3)–O(4)	103.8	O(4)–O(6)–O(2)	55.7	O(5)–O(7)–O(1)	61.9
O(3)–O(4)–O(8)	80.3	O(6)–O(2)–O(4)	61.9	O(7)–O(1)–O(5)	58.1
O(4)–O(8)–O(7)	91.3	O(4)–O(6)–O(8)	60.0	O(1)–O(5)–O(7)	60.0
O(8)–O(7)–O(3)	77.4	O(6)–O(8)–O(4)	62.3	O(7)–O(1)–O(3)	53.7
O(1)–O(3)–O(2)	47.7	O(8)–O(4)–O(6)	57.7	O(1)–O(3)–O(7)	57.6
O(3)–O(1)–O(2)	68.7	O(6)–O(8)–O(5)	52.8	O(3)–O(7)–O(1)	68.7
O(3)–O(2)–O(1)	63.6	O(8)–O(5)–O(6)	59.5		

[a] Standard deviations, 0.02–0.04 Å. [b] Standard deviations, 2.0–3.0°.

distance. The average O–O separation in a ring (the "bite" of the ring) is 2.781 Å. This is comparable to the values of 2.80 Å found in $Y(C_5H_7O_2)_3 \cdot 3H_2O$[5] and 2.778 Å for the average of the 16 chelates surveyed by Lingafelter and Braun.[12]

The mean deviations of the carbon and oxygen atoms from the unweighted least-squares planes of the acetylacetonate groups are 0.014, 0.084, and 0.015 Å for the groups containing O(1)–O(2), O(3)–O(4), and O(5)–O(6), respectively. The distances of the lanthanum ion from these planes are 0.09 ± 0.02, 0.57 ± 0.11, and 0.05 ± 0.02 Å, respectively. The metal–chelate rings containing O(1)–O(2) and O(5)–O(6) are essentially planar; the sums of the interior angles are 721.0 and 719.6°, as compared with 720° required for planarity. The sum of the interior angles for the ring containing O(3)–O(4) is 711.5°, and this ring is folded by 15.6° about the O(3)–O(4) line away from the water molecules toward the ring containing O(1)–O(2).

The coordination polyhedron formed by the eight oxygen atoms about a lanthanum ion may be described as a distorted square antiprism. Figure 2 shows the polyhedron viewed along the axis from the lanthanum ion to the center of the quadrilateral O(1)–O(2)–O(5)–O(6). The distances and angles of the polyhedron are listed in Table IV. In addition to the distortions in lengths and angles, the quadrilateral O(3)–O(4)–O(8)–O(7) is folded about the O(3)–O(8) diagonal by 26°.

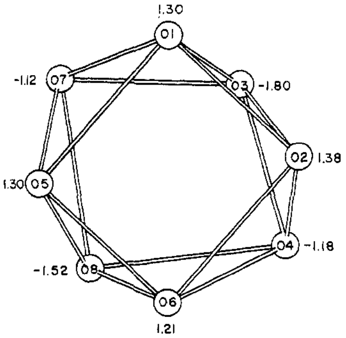

Figure 2.—Coordination polyhedron formed by the eight oxygens bonded to lanthanum. The distance of each atom from the central plane is given.

Although there is considerable deviation from the idealized $\bar{8}2m$ symmetry, the average parameters for this polyhedron agree with those of Hoard and Silverton[13] based on the minimization of ligand repulsive energy. In the notation of Hoard and Silverton, we have l = 1.253, s = 1.179, l/s = 1.063, and θ = 57.1°, as compared with their ideal values of 1.258, 1.190, 1.057, and 57.3°. The distortion of the square antiprism may be attributed to the presence of chemically different ligands bonded to the same metal atom. It should be noted that the structure could also be described as a distorted rhombic dodecahedron, since the two polyhedra can be continuously transformed into each other, and an intermediate form may even be expected if steric constraints are minimized by the presence of a large cation. Our description is based on the simple observation that Figure 2 looks like a square antiprism.

Distances suggestive of hydrogen bonding are O(7)–O(1)′ = 2.770 Å, O(7)–O(5)′ = 2.836 Å, O(8)–O(4)″ = 2.757 Å, O(8)–O(6)″ = 2.768 Å, where the primes indicate atoms related to the unprimed atoms by the center of symmetry at the origin and the double primes indicate atoms related by the center of symmetry at $^1/_2$, $^1/_2$, $^1/_2$. The O(7)–O(7)′ distance is 3.029 Å. The molecules are thus linked by hydrogen bonds in zigzag chains which are very nearly parallel to the [101] direction. The longest dimension of the crystals is parallel to this direction. No close contacts exist between the chains, and the shortest interchain distance is 3.39 Å between O(7) and C(14). Careful consideration of the scheme of hydrogen bonding suggests that the hydrogen positions in Table II are not reliable.

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(13) J. L. Hoard and J. V. Silverton, *Inorg. Chem.*, **2**, 235 (1963).